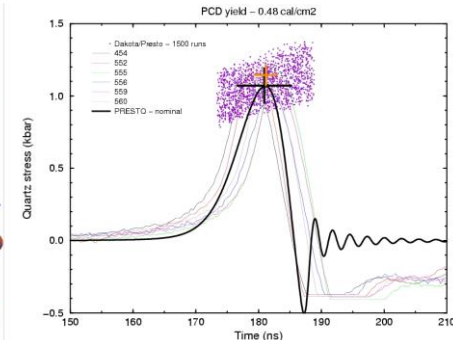
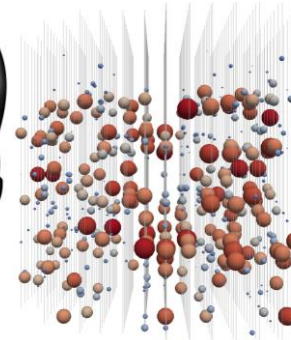
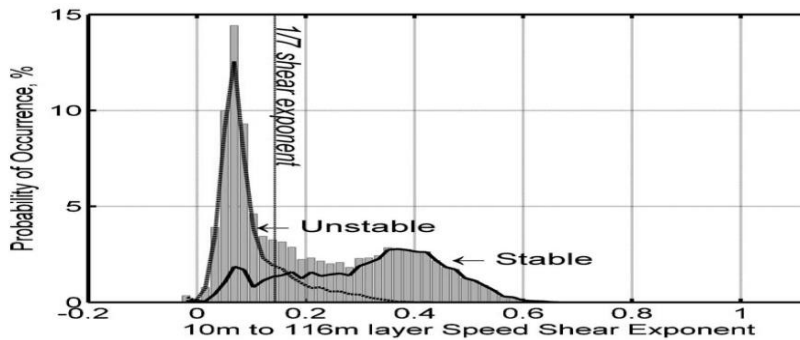


Exceptional service in the national interest



Dakota Sensitivity Analysis and Uncertainty Quantification, with Examples

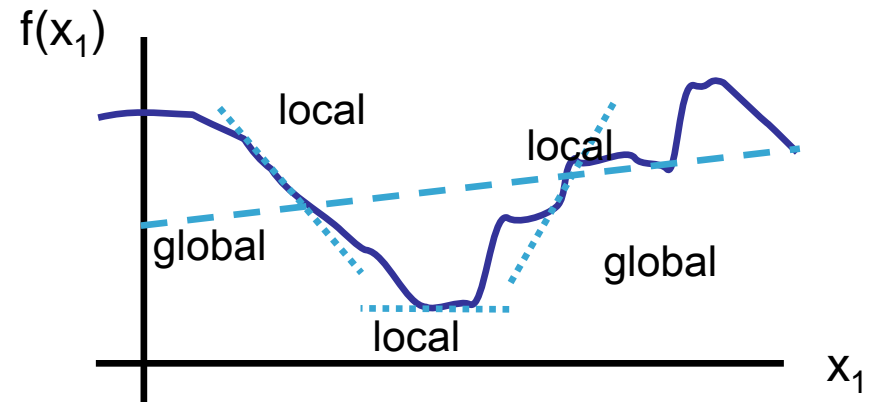
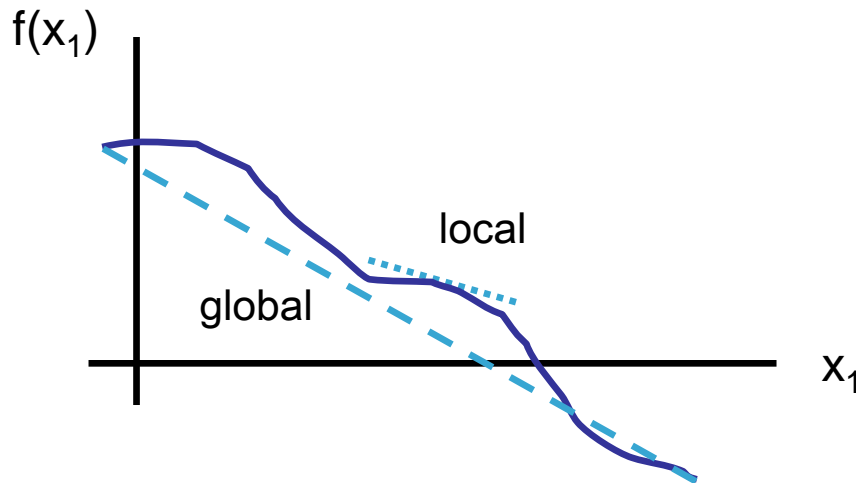
Dakota Sensitivity Analysis (SA)

- SA goals and examples
- Global SA approaches and metrics available in Dakota
- Select Dakota examples for parameter studies and global SA

Why Perform Sensitivity Analysis?

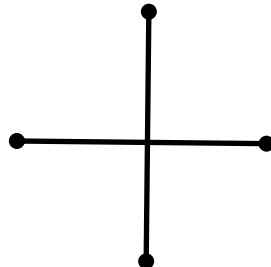
- What? Understand code output variations as input factors vary
- Why? Identify most important variables and their interactions
 - Identify key model characteristics: smoothness, nonlinear trends, robustness
 - Provide a focus for resources
 - Data gathering and model development
 - Code development
 - Uncertainty characterization
 - Screening: Identity the most important variables, down-select for further UQ or optimization analysis
 - Can have the side effect of identifying code and model issues
 - Data can be used to construct surrogate models
- Dakota SA formalizes and generalizes one-off sensitivity studies you're likely already doing
- Provides richer global sensitivity analysis methods

Sensitivity Analysis: Influence of Inputs on Outputs



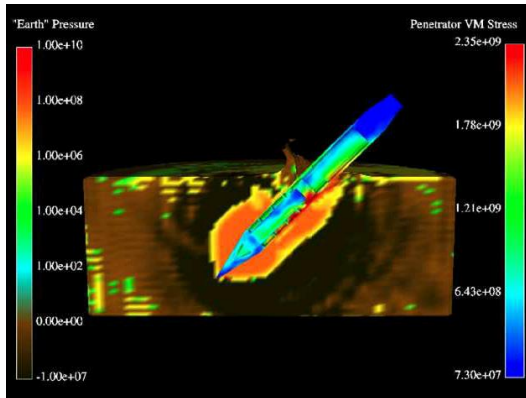
Assess variations in $f(x_1)$ due to (small or large) perturbations in x_1 .

- Local sensitivities
 - Partial derivatives at a specific point in input space.
 - Given a specific x_1 , what is the slope at that point?
 - Can be estimated with finite differences
- **Global sensitivities**
 - Found via sampling and regression.
 - What is the general trend of the function over all values of x_1 ?
 - Typically consider inputs uniformly over their whole range



many already do
basic SA;
perturb from
nominal, see effect

Global Sensitivity Analysis Example: Earth Penetrator



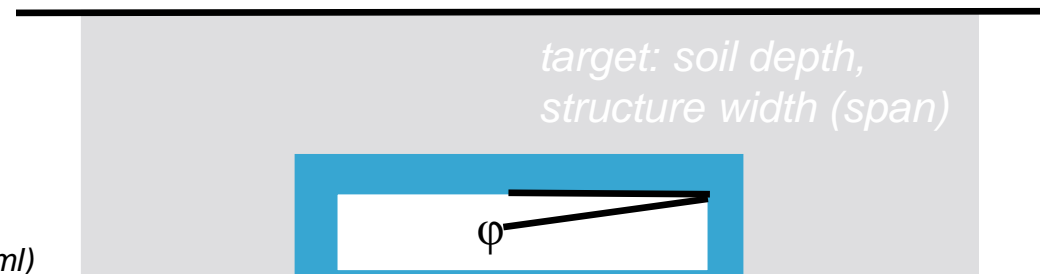
Notional model for illustration purposes only

(<http://www.sandia.gov/ASC/library/fullsize/penetrator.html>)

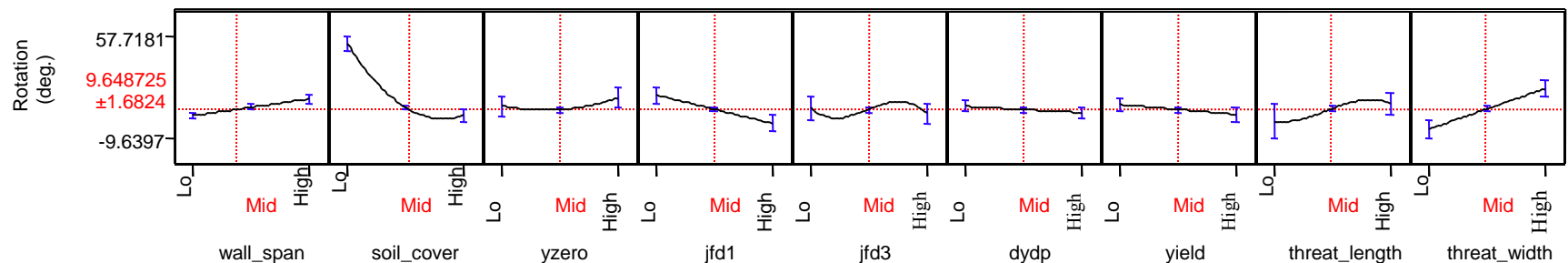
*12 parameters describing target & threat
uncertainty, including...*



threat: width, length



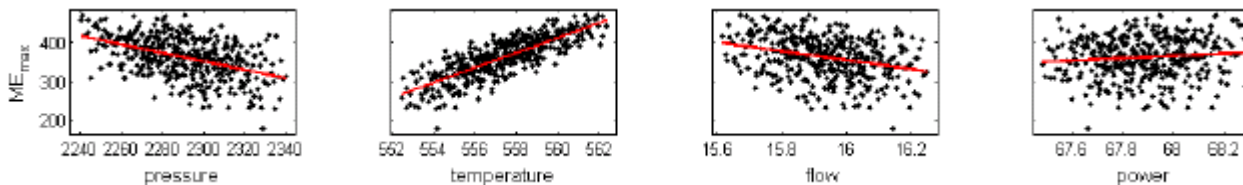
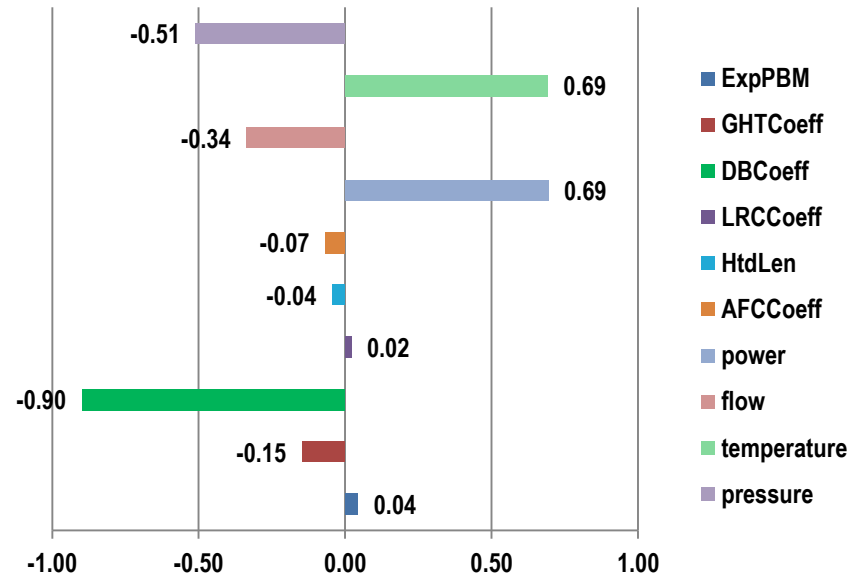
- **Underground target with external threat:** assess sensitivity in target response to target construction and threat characteristics
- Response: angular rotation (ϕ) of target roof at mid-span
- Analysis: CTH Eulerian shock physics code; JMP stats
- Revealed most sensitive input parameters and nonlinear relationships



Global SA Example: Nuclear Reactor Thermal-Hydraulics Model

- Assess parameter influence on boiling rate, a key crud predictor
- Dakota correlation coefficients: strong influence of **core operating parameters** (pressure more important than previously thought)
- **Dittus-Bolter** correlation model may dominate model form sensitivities (also nonlinear effects of **ExpPBM**)
- Scatter plots help visualize trend in input/output relationships

parameter influence on number of boiling sites



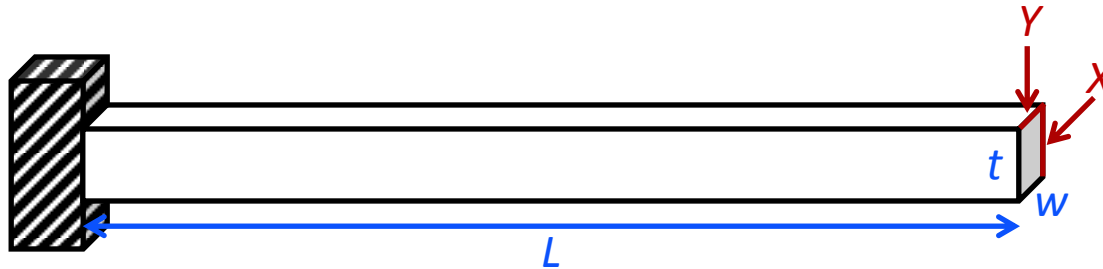
sensitivity of mass evaporation rate (max) to operating parameters

Group Discussion Questions:

Your Sensitivity Analysis Practice

- Do you currently perform sensitivity analysis or parameter perturbations?
- What are example SA questions you (could) ask in your domain?
- How do (would) you answer them?
- What measures of sensitivity, ranking, or importance are you most familiar with?
- What are the key challenges you face?

Cantilever Beam Model



Parameters:

L : length (in)

w : width (in)

t : thickness (in.)

ρ : density (lb/ft³)

E : Young's modulus (lb/in²)

X : horizontal load (lb)

Y : vertical load (lb)

Responses:

M : mass (lb)

S : stress (lb/in²)

D : displacement (in)

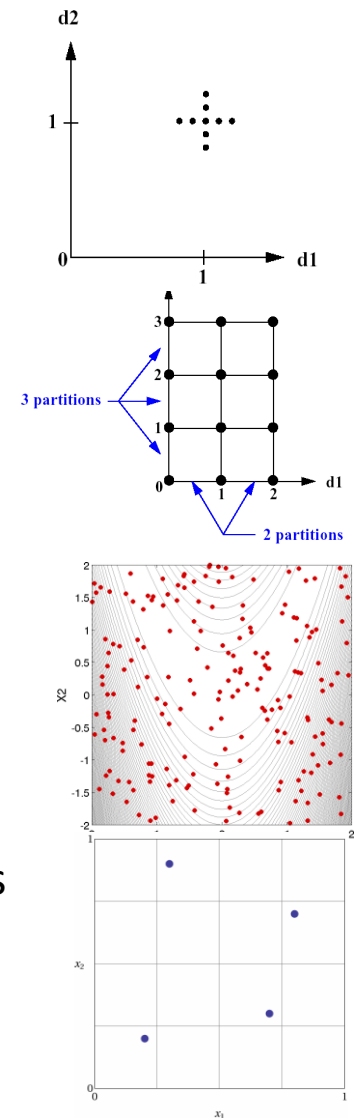
$$M = \rho * wt * \frac{L}{12^3}$$

$$S = \frac{600}{wt^2} Y + \frac{600}{w^2 t} X$$

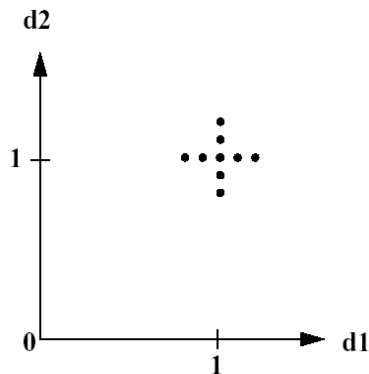
$$D = \frac{4L^3}{Ewt} \sqrt{\left(\frac{Y}{t^2}\right)^2 + \left(\frac{X}{w^2}\right)^2}$$

Global Sensitivity Analysis in Dakota

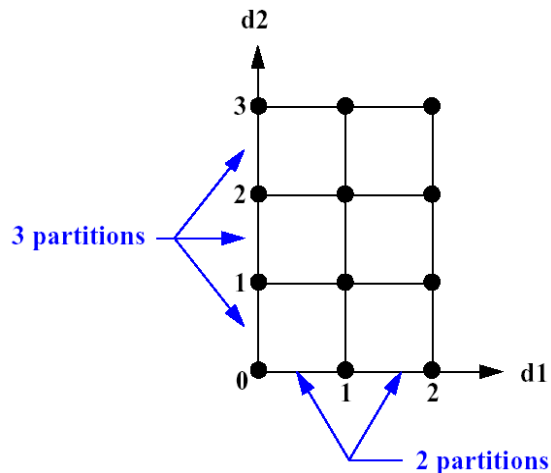
- Assess effect of input variables considered jointly over their whole range. Dakota process:
 - **Specify variables:** lower and upper bounds
 - **Specify method:** e.g., uniform random sampling
 - **Specify responses:** compute response value at each sample point
 - **Run Dakota and analyze** input/output relationships
- **Sample designs** (methods) available:
 - Parameter studies: list, **centered**, **grid**, vector, user
 - Random sampling: Monte Carlo, **Latin hypercube**, Quasi-MC, CVT
 - DOE/DACE: Full-factorial, orthogonal arrays, Box-Behnken, CCD
 - **Morris one-at-a-time**
 - Sobol indices via variance-based decomposition, polynomial chaos
- **Metrics:** trends, correlations, main/interaction effects, Sobol indices, importance factors/local sensitivities



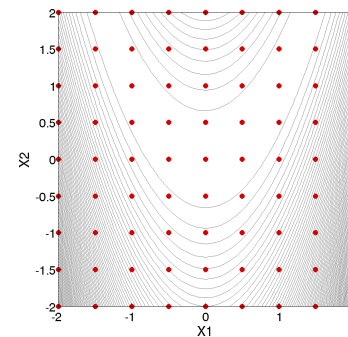
Basic Dakota SA for Cantilever: Centered and Grid Parameter Studies



- Start at nominal values, perturb up and down in each coordinate direction
- Specify the parameter variations, which responses to study
- See Dakota input and output (following slides)



- What changes to Dakota input will instead perform the **grid parameter study** at left?
- Dakota Reference Manual helps with keyword choice...
- What are benefits/drawbacks of these methods?



*Example:
uniform grid
over [-2.0, 2.0]*

Dakota Input File: Cantilever Centered Parameter Study

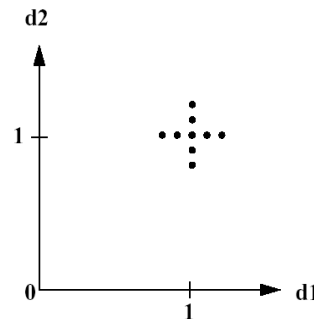
```
environment
  tabular_data output_precision 1e-16
```

```
method
  centered_parameter_study
    step_vector 0.1 0.1 2.0
              10 1.e5 5. 10.
    steps_per_variable 2
```

```
variables
  active all
  continuous_design = 3
    initial_point 2*1.0 20.0
    descriptors "w" "t" "L"
  continuous_state = 4
    initial_state 500. 29.E+6 50. 100.
    descriptors 'p' 'E' 'X' 'Y'
```

```
interface,
  fork
    analysis_driver = 'driver.sh'
```

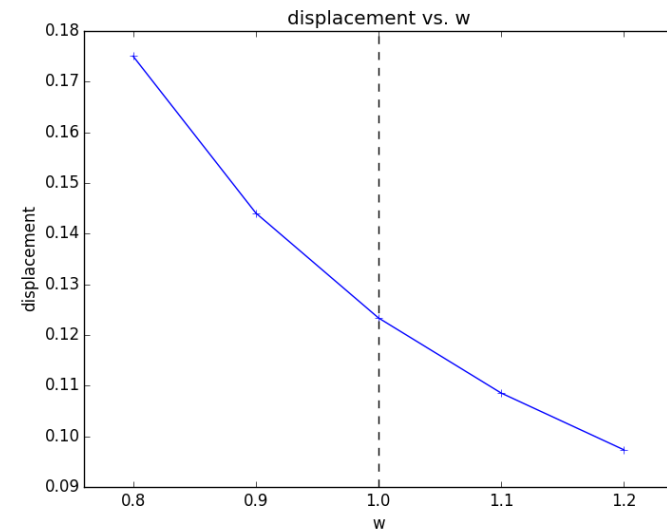
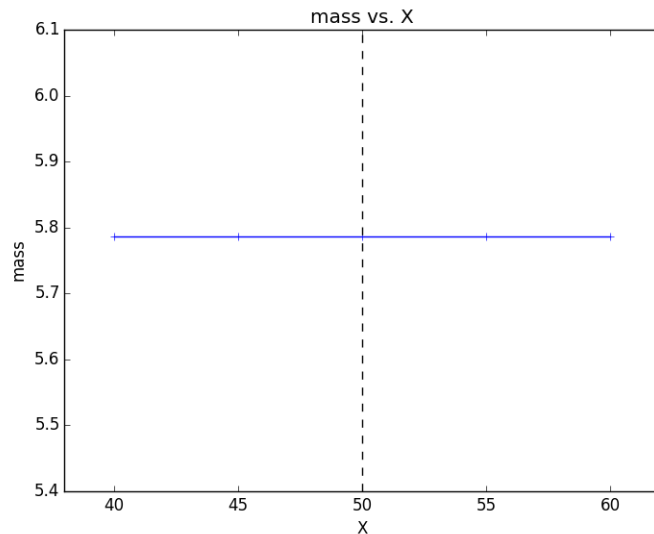
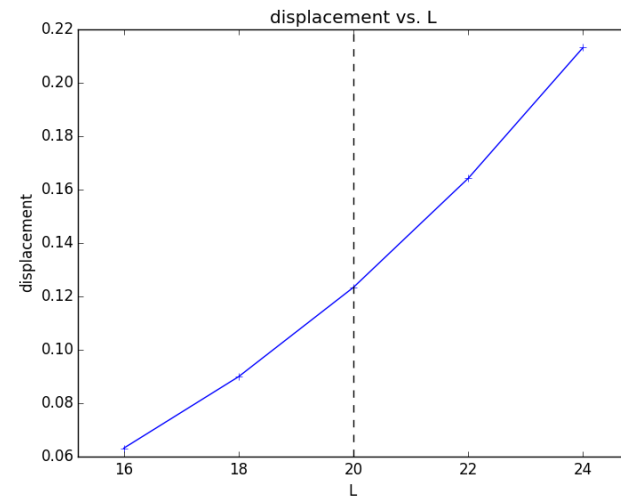
```
responses,
  num_objective_functions = 3
    response_descriptors = 'mass' 'stress' 'displacement'
  no_gradients
  no_hessians
```



- Catalog variable/response sets to tabular file
- Algorithm configuration: steps in each variable
- Center point: initial point / initial state
- How parameters are mapped to responses
- Responses from simulation

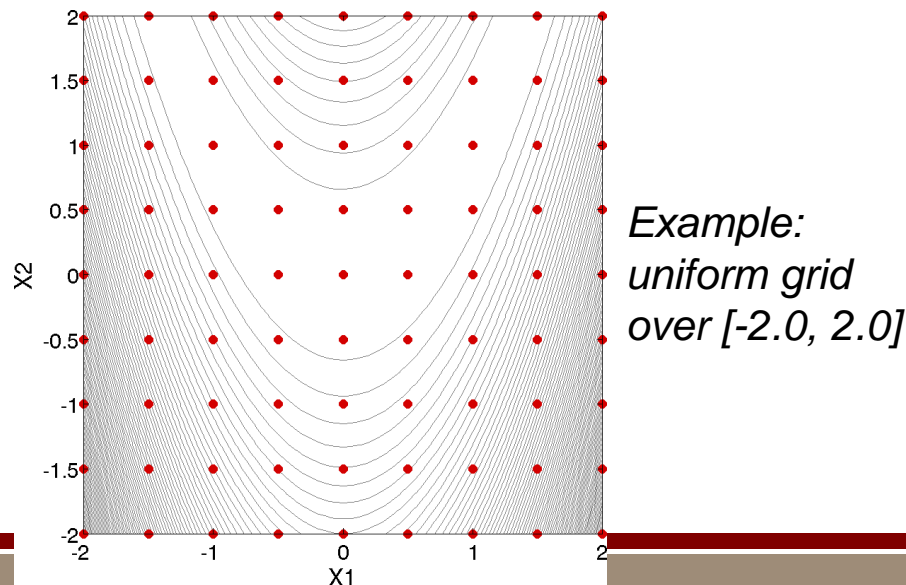
Results: Centered Parameter Study

- Python plots of Dakota tabular file
- Univariate effects of parameters on each response
- What do you observe?
- What are benefits/drawbacks?



Exercise: Multi-dimensional Parameter Study

- Goal: understand how responses *area*, *stress*, and *displacement* vary with respect to the inputs *w* and *t* on a grid of points.
- Exercise: change previous input file to run the *mod_cantilever* computational model at a grid of points over $[1.0, 4.0]$ using the *multidim_parameter_study* method
- Try 9 points in one dimension, 6 in the other
- See method and variable commands in Dakota reference manual
- What parts of the file did you have to change?



Dakota Input File and Results: Cantilever Multi-dimensional Parameter Study

```
environment
  tabular_data output_precision 1e-16
```

```
method
```

```
  multidim_parameter_study
    partitions = 2 2 2 2 2 2
```

```
variables
```

```
  active all
  continuous_design = 3
```

```
  upper_bounds = 1.2 1.2 6.0
  lower_bounds = 0.8 0.8 4.0
```

```
  descriptors      "w"      "t"      "L"
  continuous_state = 4
```

```
  upper_bounds = 600. 35.E+6 60. 120.
  lower_bounds = 400. 23.E+6 40. 80.
```

```
  descriptors      'p'      'E'      'X'      'Y'
```

```
interface,
```

```
fork
```

```
  analysis_driver = 'driver.sh'
```

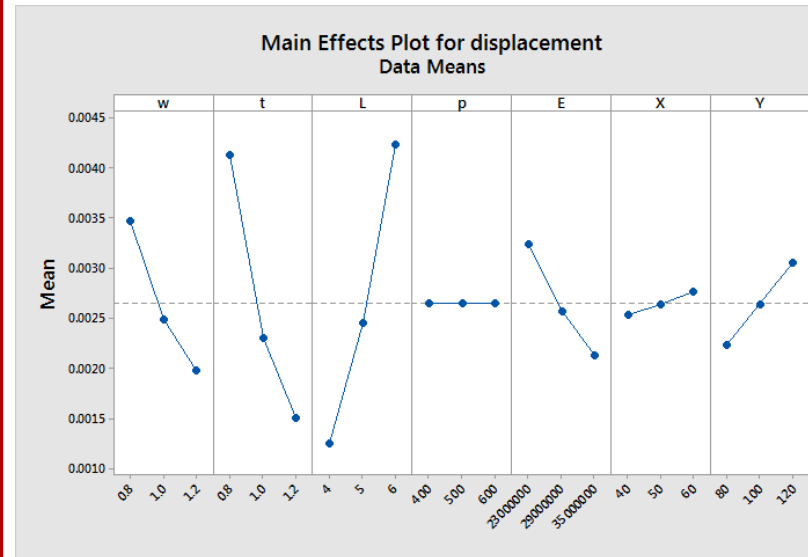
```
responses,
```

```
num_objective_functions = 3
```

```
  response_descriptors = 'mass' 'stress' 'displacement'
```

```
no_gradients
```

```
no_hessians
```

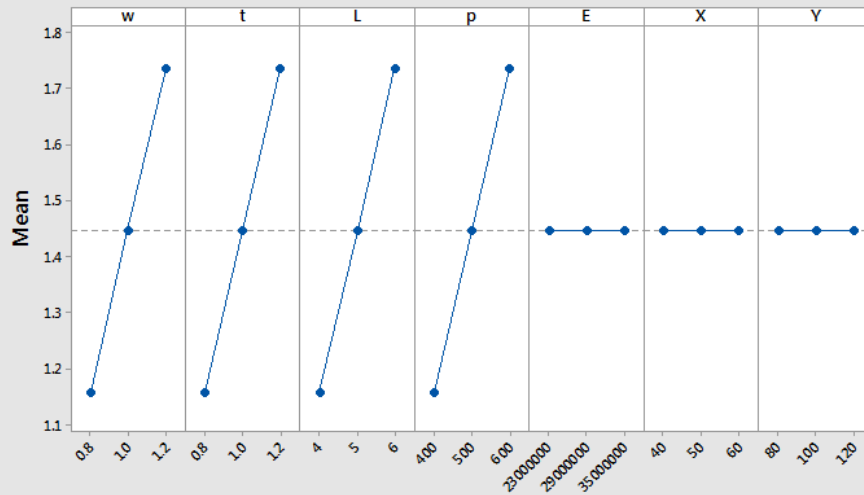


Dakota tabular data plotted with Minitab

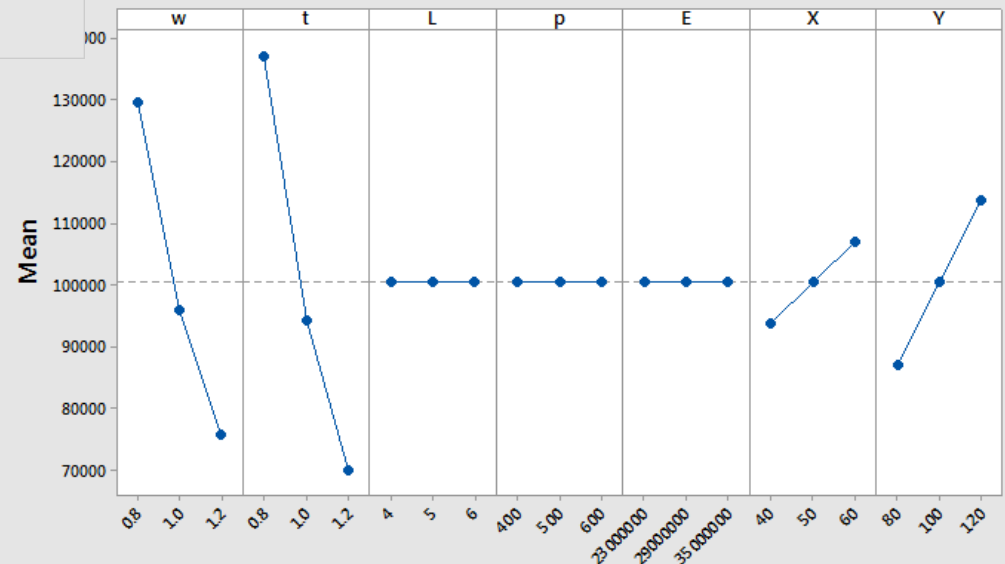
What are benefits/drawbacks?

Dakota Input File and Results: Cantilever Multi-dimensional Parameter Study

Main Effects Plot for mass
Data Means

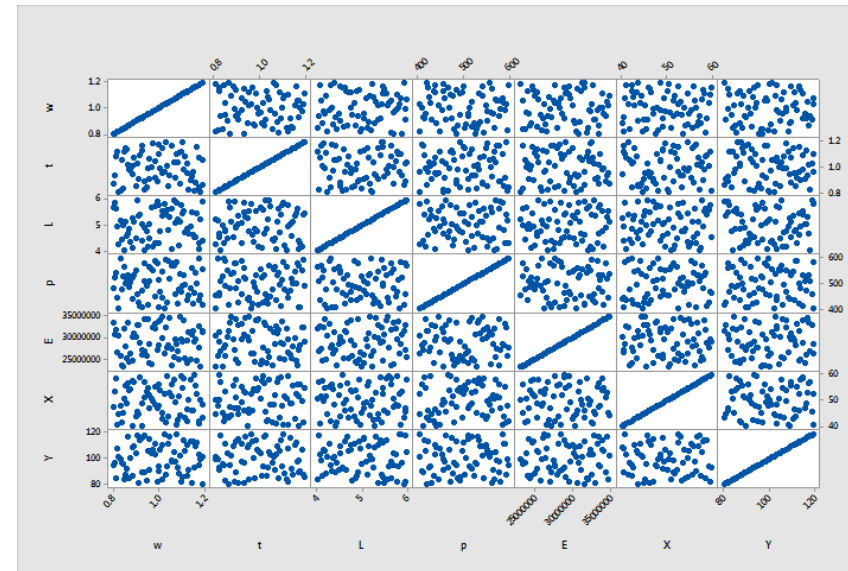


Main Effects Plot for stress
Data Means



Workhorse SA Method: Random Sampling

- Generate space filling design (typically Monte Carlo or Latin hypercube with samples = 2x or 10x number of variables)
- Run model at each point
- Analyze input/output relationships with
 - Correlation coefficients
 - Simple correlation: strength and direction of a linear relationship between variables
 - Partial correlation: like simple correlation but adjusts for the effects of the other variables
 - Rank correlations: simple and partial correlations performed on “rank” of data
 - Regression and resulting coefficients
 - Variance-based decomposition
 - Importance factors



Two-dimensional projections
of LHD for Cantilever
(plotted with Minitab)

Dakota Input File: Cantilever LHS Study

```
method
  sampling
  sample_type lhs
  samples = 70
  seed = 3845

variables
  active all
  continuous_design = 3
    upper_bounds = 1.2 1.2 6.0
    lower_bounds = 0.8 0.8 4.0
    descriptors   "w"      "t"      "L"
  continuous_state = 4
    upper_bounds = 600. 35.E+6 60. 120.
    lower_bounds = 400. 23.E+6 40. 80.
    descriptors   'p'      'E'      'X'      'Y'

interface
  fork
    analysis_driver = 'driver.sh'

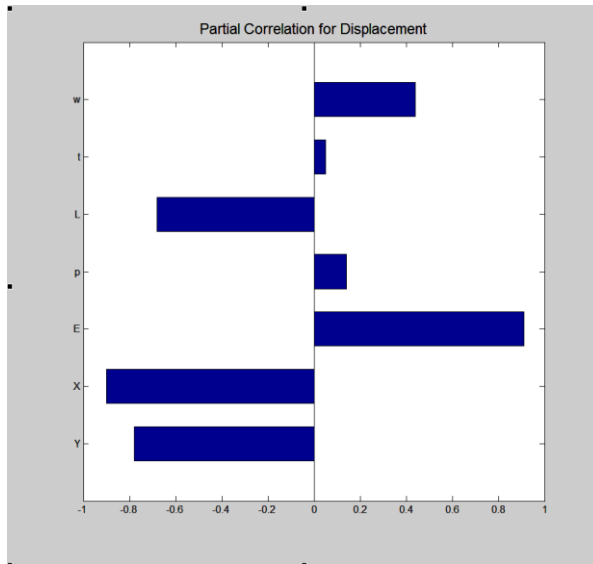
responses
  response_functions = 3
  descriptors = 'mass' 'stress' 'displacement'
  no_gradients no_hessians
```

Global Sampling Results for Cantilever

Partial Correlation Matrix for Cantilever

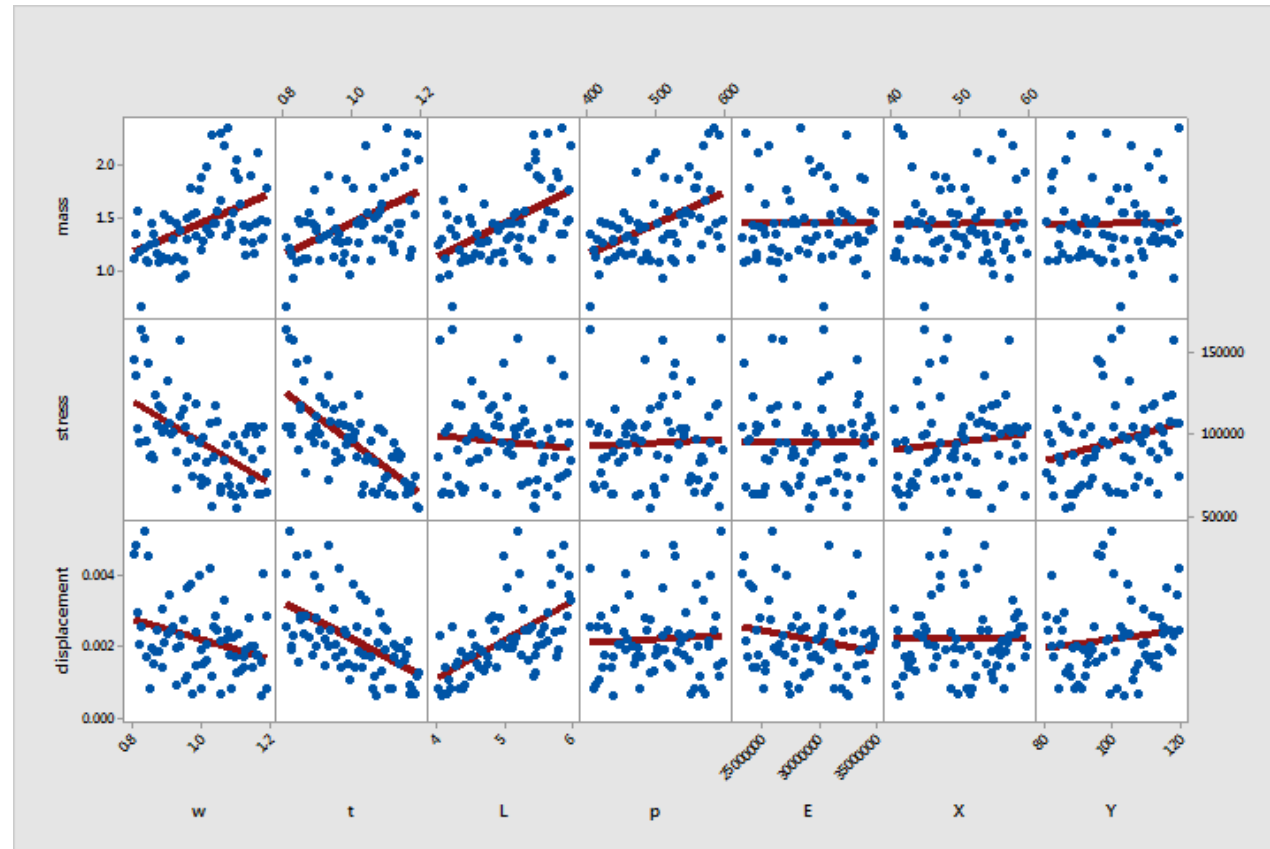
	mass	stress	displacement
w	0.95	-0.96	-0.78
t	0.95	-0.97	-0.90
L	0.96	-0.17	0.91
p	0.95	0.11	0.14
E	-0.08	-0.13	-0.68
X	-0.03	0.54	0.05
Y	0.12	0.82	0.44

correlation coefficients
from Dakota console
output (colored w/ Excel)



(plotted with Matlab)

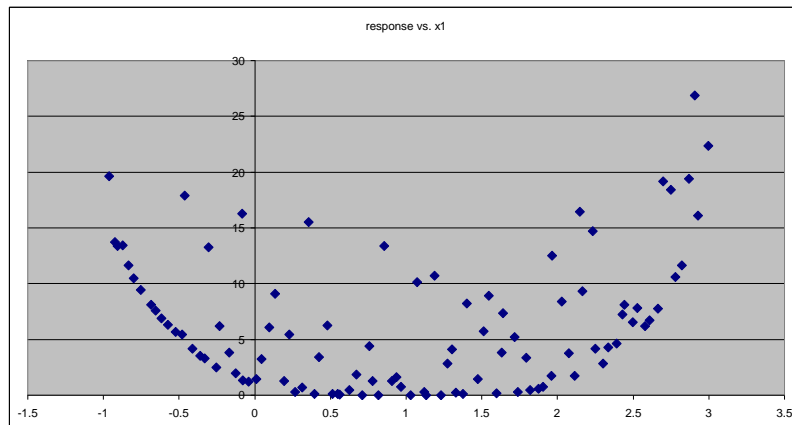
Dakota tabular data plotted in Minitab (can use Matlab, JMP, Excel, etc.)



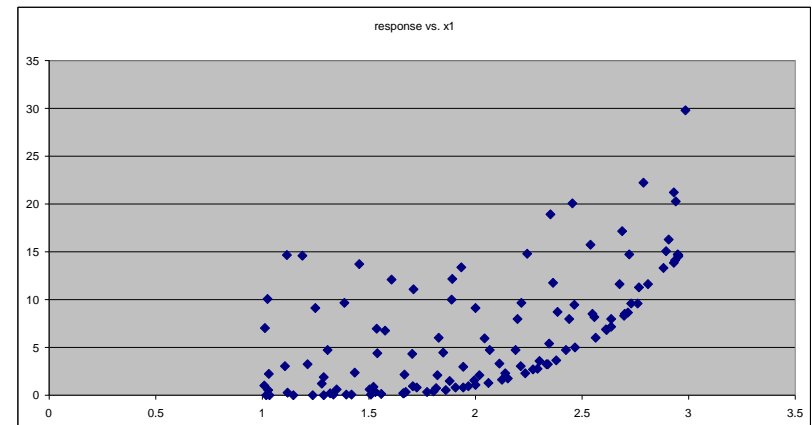
Group discussion

- What is expected, limited about this approach?
- What approaches would you take?
- What assumptions are we making? How would changing them affect results?

Bounds = [-1, 3]

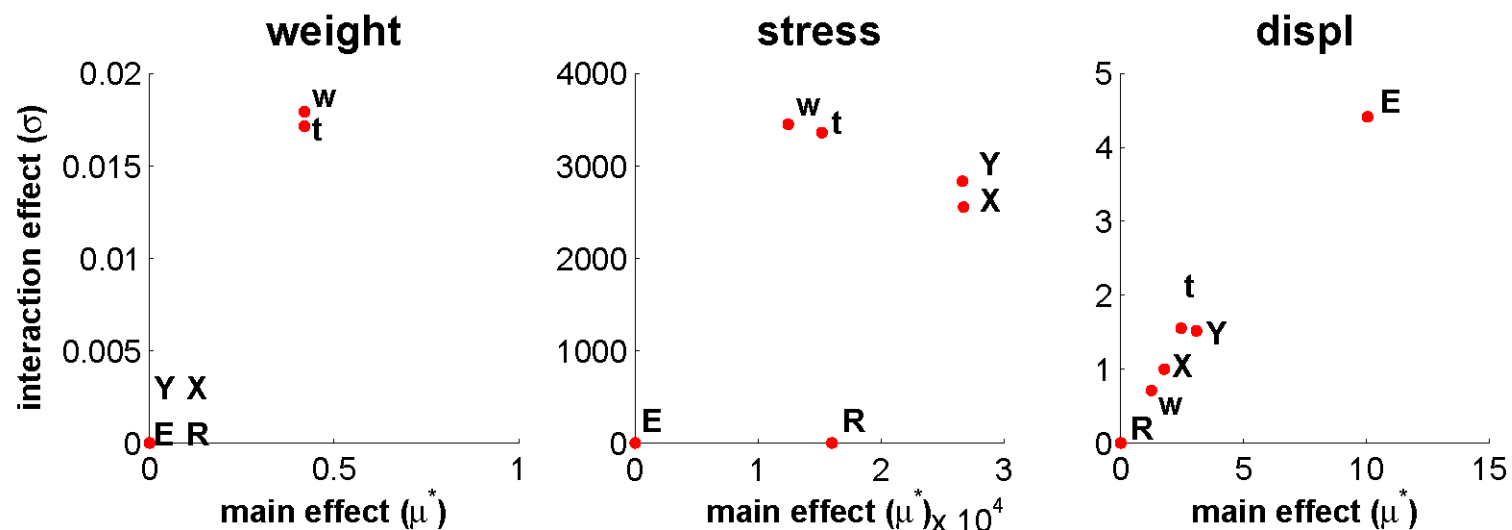


Bounds = [1, 3]



Morris One-at-a-Time (MOAT)

- Sample paths around global space in coordinate directions
- Give good measure of main (linear, first-order) and interaction / nonlinear effect for modest simulation budget
- How would you know how to configure Dakota to do this study?



Other SA Approaches Require Changing Method

- Dakota Reference Manual guides in specifying keywords

```
method,  
sampling  
  sample_type lhs  
  seed =52983  
  samples = 100
```

LHS Sampling

```
method,  
  dace oas  
  main_effects  
  seed =52983  
  samples = 500
```

Main Effects Analysis using
Orthogonal Arrays

```
method,  
sampling  
  sample_type lhs  
  seed =52983  
  samples = 500  
  variance_based_decomp
```

Variance-based Decomposition
using LHS Sampling

```
method,  
  psuade_moat  
  partitions = 3  
  seed =52983  
  samples = 100
```

Morris One-At-a-Time

Dakota Sensitivity Analysis Summary

- What? Understand code output variations as input factors vary; main effects and key parameter interactions.
- Why? Identify most important variables and their interactions
- How? What Dakota methods are relevant? What results?

Category	Dakota method names	univariate trends	correlations	modified mean, s.d.	main effects Sobol inds.	importance factors / local sensis
Parameter studies	centered, vector, list	P				
	grid		D		P	
Sampling	sampling, dace lhs, dace random, fsu_quasi_mc, fsu_cvt with variance_based_decomp...	P	D		D	
DACE (DOE-like)	dace {oas, oa_lhs, box_behnken, central_composite}		D		D	
MOAT	psuade_moat			D		
PCE, SC	polynomial_chaos, stoch_collocation				D	D
Mean value	local_reliability					D

multi-purpose!

D: Dakota
P: Post-processing
(3rd party tools)

- Also see Dakota Usage Guidelines in User's Manual

Sensitivity Analysis References

- Saltelli A., Ratto M., Andres T., Campolongo, F., et al., *Global Sensitivity Analysis: The Primer*, Wiley, 2008.
- J. C. Helton and F. J. Davis. Sampling-based methods for uncertainty and sensitivity analysis. Technical Report SAND99-2240, Sandia National Laboratories, Albuquerque, NM, 2000.
- Sacks, J., Welch, W.J., Mitchell, T.J., and Wynn, H.P. Design and analysis of computer experiments. *Statistical Science* 1989; 4:409–435.
- Oakley, J. and O’Hagan, A. Probabilistic sensitivity analysis of complex models: a Bayesian approach. *J Royal Stat Soc B* 2004; 66:751–769.
- Dakota User’s Manual
 - Parameter Study Capabilities
 - Design of Experiments Capabilities/Sensitivity Analysis
 - Uncertainty Quantification Capabilities (for MC/LHS sampling)
- Corresponding Reference Manual sections